Nanoscale Engineering of Heat Transfer and Energy Conversion Processes

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? What Can Be Engineered? ? Phonon and Electron Transport. ? Engineering Photon Properties.

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OUTLINE

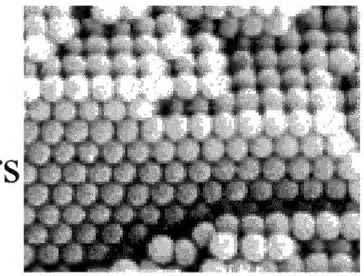
- What Can Be Engineered?
- Phonon and Electron Transport.
- Engineering Photon Properties.

HISTORY OF ENGINEERED STRUCTURES

- **Photons:**

Nature Given: Free Space Propagating Wave

Engineered: Interference Filters and Coatings, >100 Years
Photonic Crystals, 2D and 3D, ~15 Years

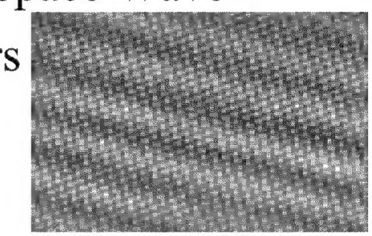


(Baughman et al., 2000)

- **Electrons:**

Nature Given: Inside Solids, Band Formation, 3D, or Free Space Wave

Engineered: Quantum Wells, Superlattices, 2D, ~30 Years
Quantum Wires, Quantum Dots, 1D, 0D
Quantum Dot Superlattices, 3D



- **Phonons:**

Nature Given: Inside Solids, Band Formation, 3D, or Free Space Wave

Engineered: Phonon Filters: 1D, ~20 Years (Low Temperature)
Phononic Crystals: 3D ~10 Years (Long Wavelength)
Quantized Transport, Recent (Very Low Temperature)

CONDITIONS FOR ENGINEERING

- **WAVE REGIME   Phase Preservation**

  Long Mean Free Path for Phase Preservation
  Hetero-Interfaces for Phase Addition/Subtraction
  (a) Wavelength Comparable to Unit Cell (Zero's Order Effect)
  (b) Wavelength Much Longer than Atoms: Effective Medium
  Energy Separation Larger Than Thermal Fluctuation

- **PARTICLE REGIME   Direction Change**

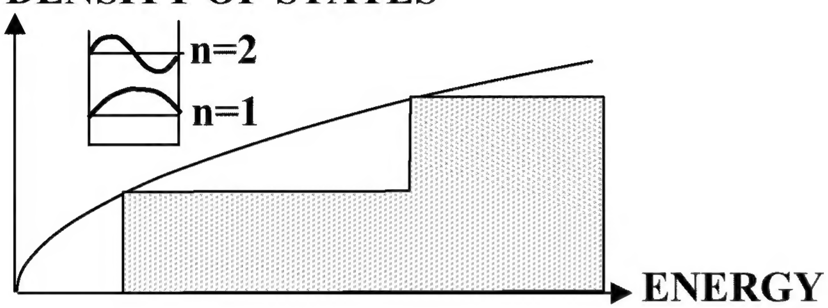
  Long Mean Free Path and Hetero-Interfaces

- **ORDER OF MAGNITUDES IN SOLIDS**

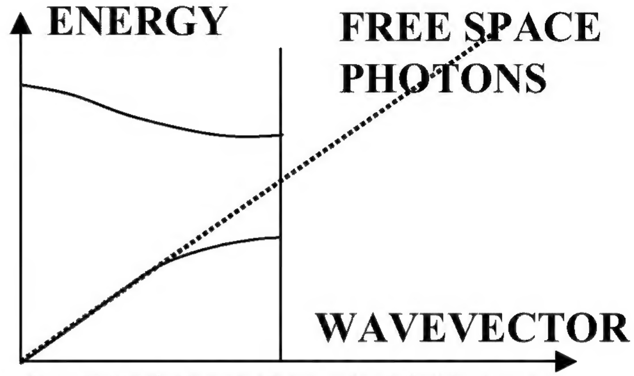
  Electron/Phonon Mean Free Path: 10 – 1000 Å
  Electron Wavelength: 10-100 Å
  Dominant Phonon Wavelength: 10-50 Å
  Photon wavelength and mean free path ~1μm and up

Nanostructures Are the Playground!!!

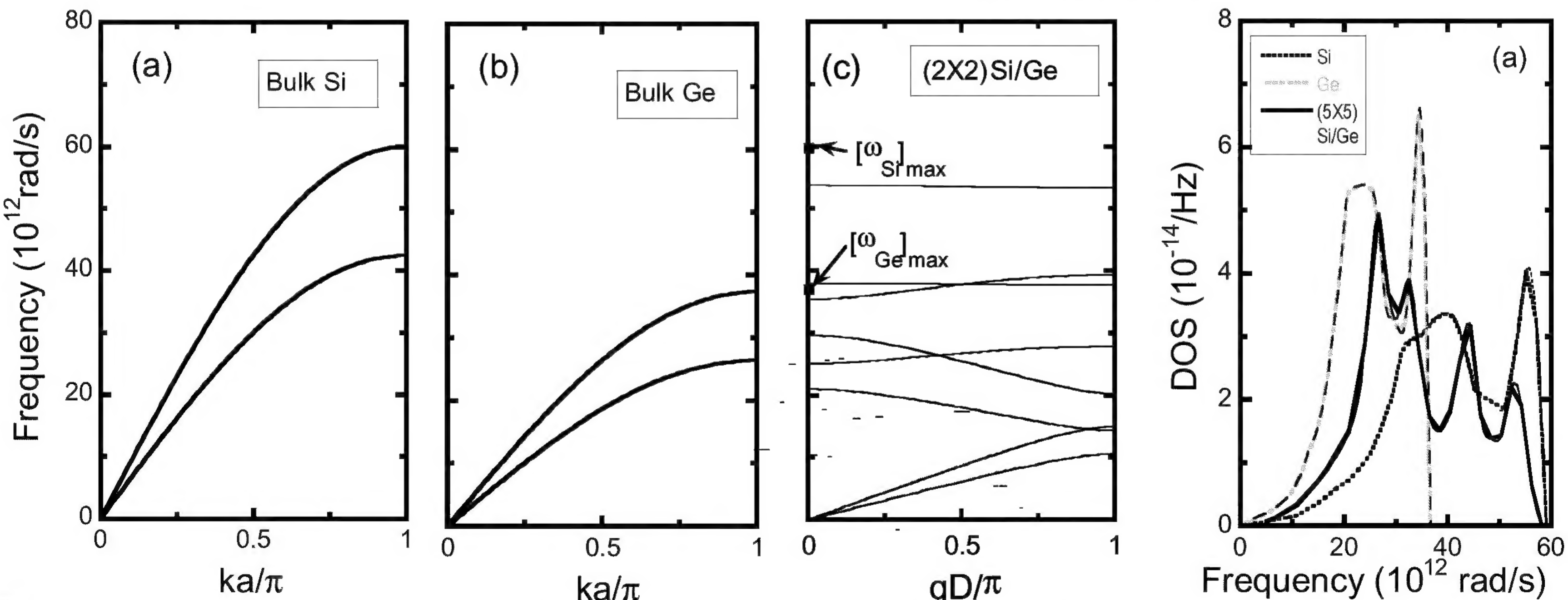
ENGINEERING ENERGY STATES



(a) ELECTRONS IN QUANTUM WELL



(b) PHOTONIC CRYSTALS



(c) PHONONS IN SUPERLATTICES

APPLICATIONS

- **Utilization of Electronic Energy State Change**

  Quantum Well Lasers: Electron Density of States Change
  Quantum Cascade Lasers: Artificial Energy Levels/Bandgaps
  Quantum Well Detectors: Artificial Energy Levels/Bandgaps

- **Utilization of Photonic Energy State Change**

  Photonic Fibers, etc.? Mostly Under Investigation but Exciting!

- **Concurrent Electron-Photon State Change**

  Microcavity Lasers, etc. Mostly Under Investigation
  Quantum Dots as Biological Tags (photoluminescence)

- **Concurrent Electron-Phonon State Change**

  Relaxation Time of Electrons for Better Lasers, Under Investigation

Wavelength Specific Application!!!

Transport Properties Nonessential!!!

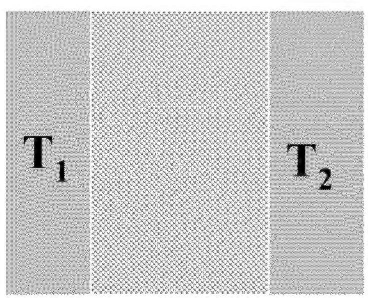
ENGINEERING THERMAL ENERGY TRANSPORT

- **KINETIC FORMULISM**

$$q_x = \int \underbrace{v_x}_{\text{Velocity}} \bullet \underbrace{E}_{\text{Energy}} \bullet \underbrace{f \bullet d^3k}_{\text{Number Density}} = \int v_x \bullet E \bullet f \bullet D(E)dE$$

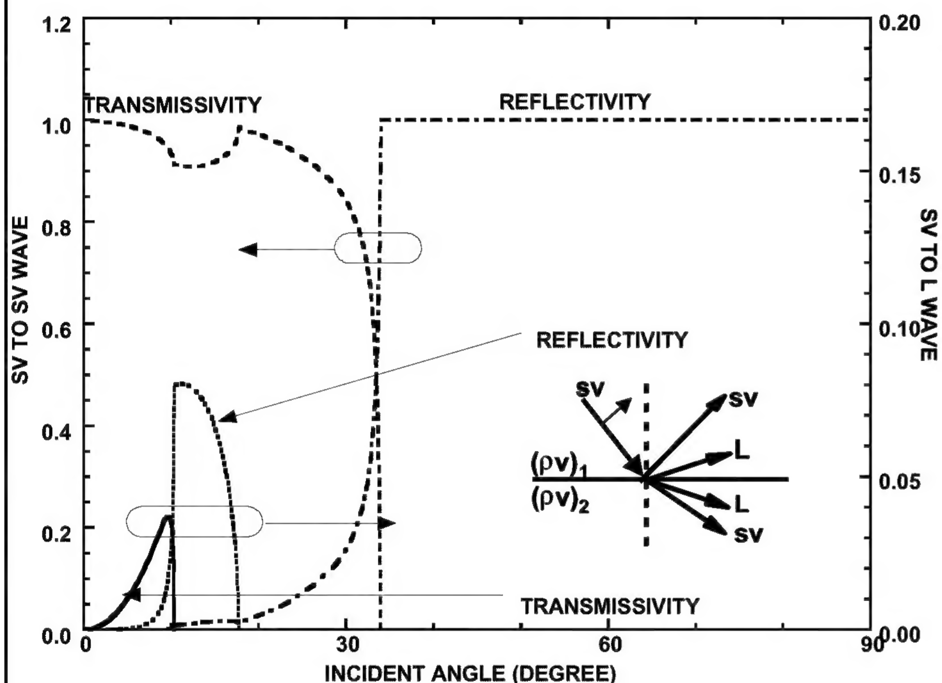
$$k = \frac{1}{3}\int v \bullet C(E) \bullet \Lambda(E)dE$$ **(Bulk Material)**

- **LANDAUER FORMULISM**

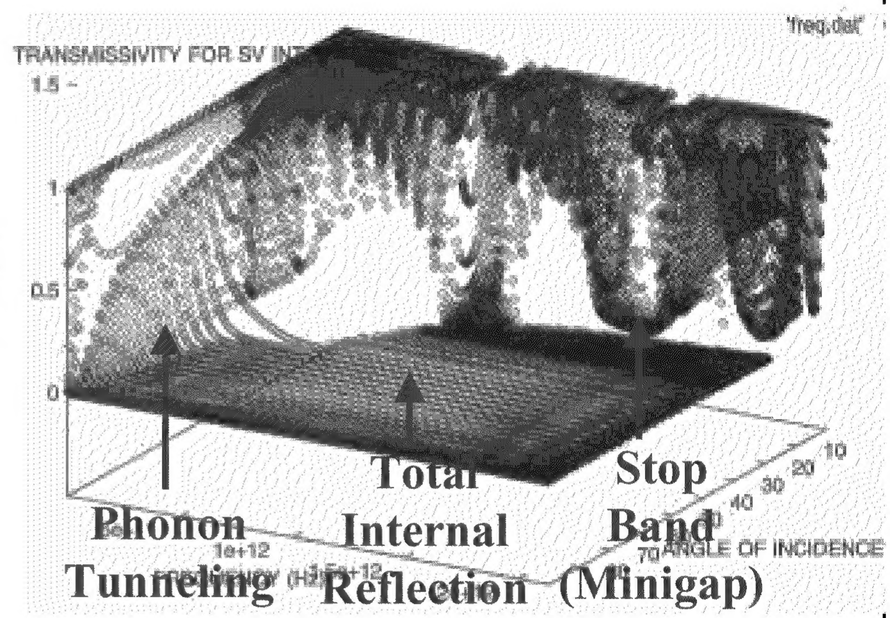


$$q_{12} = \int v_x \bullet E \bullet (f_1 - f_2) \bullet \underbrace{\tau}_{\text{Transmissivity}} \bullet d^3k$$

Phonon Transmission Cross Interfaces



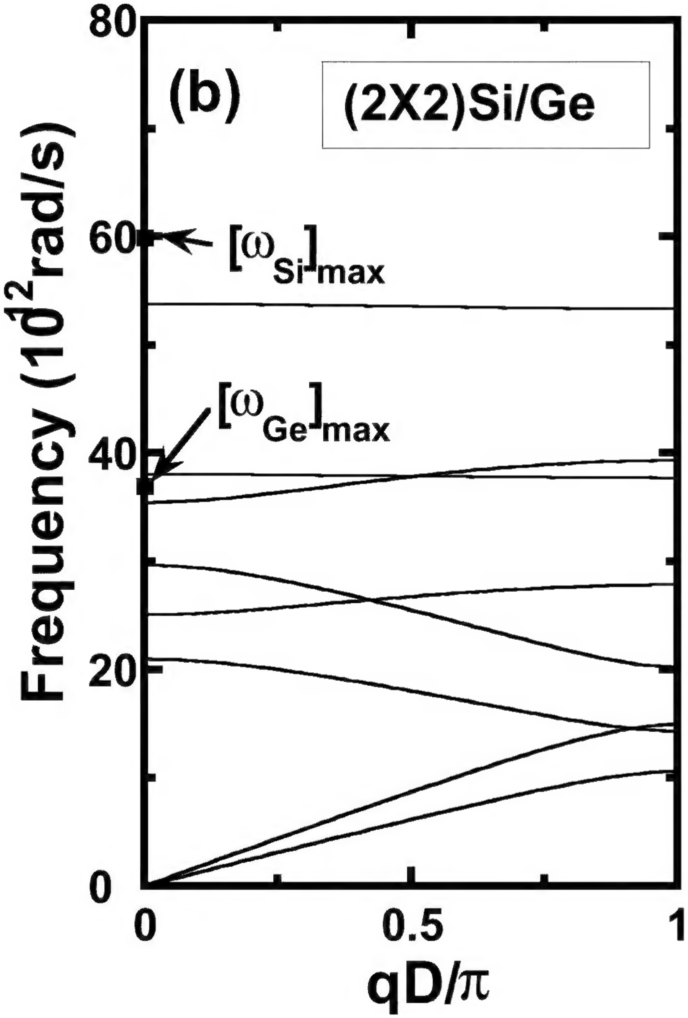
Single Interface

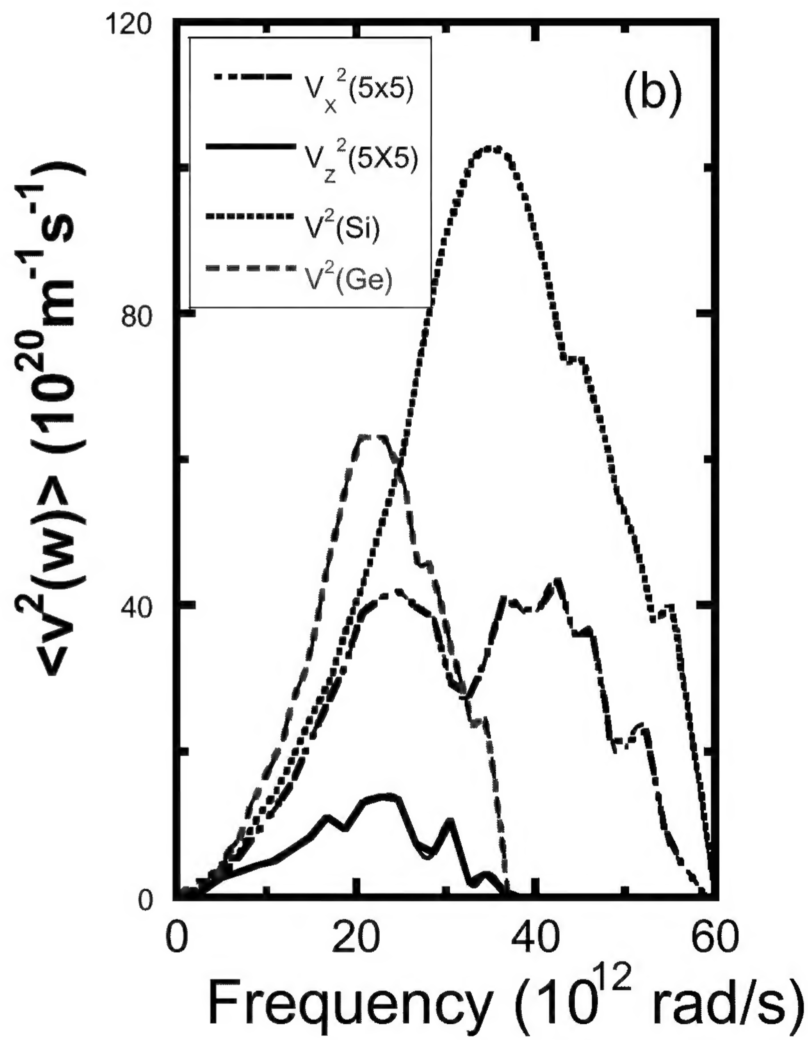


Superlattice

Chen, J. Heat Transf., 121, 945 (1999).

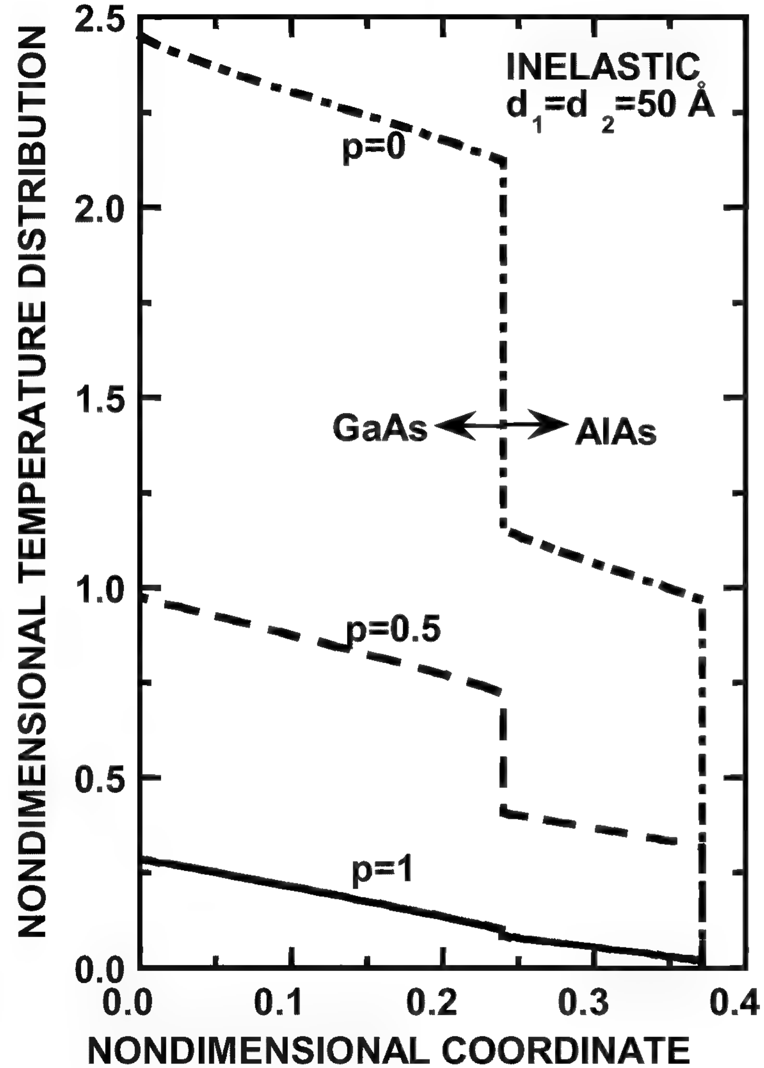
Group Velocity

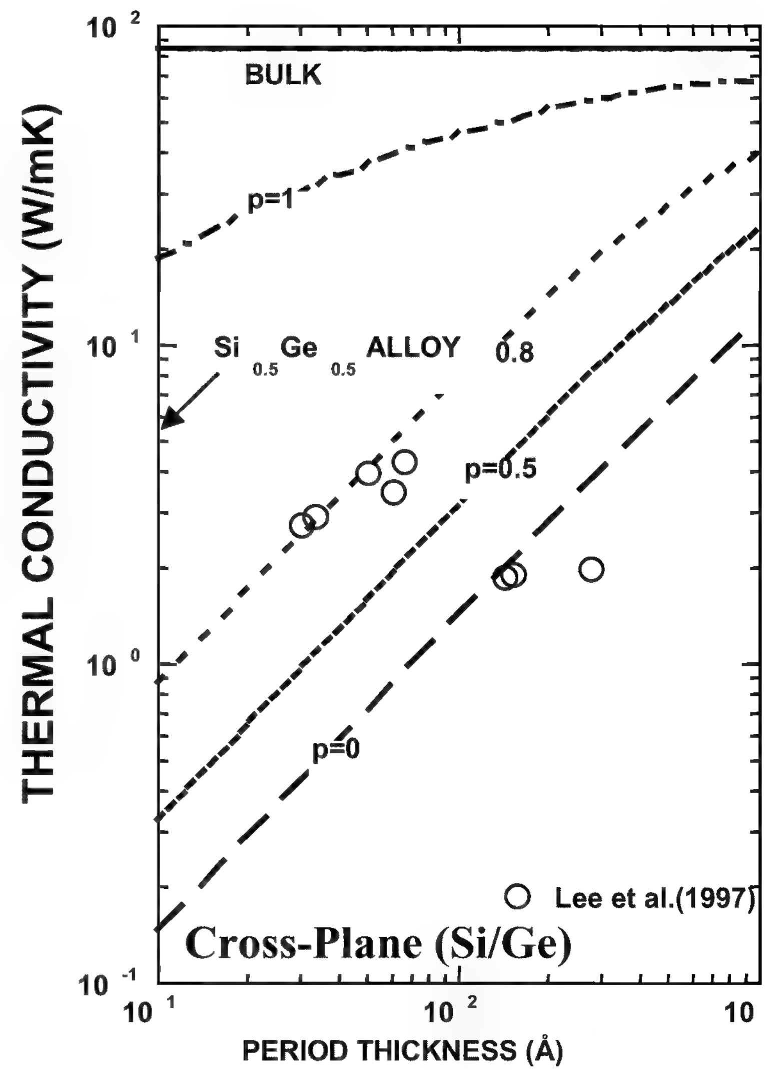




Yang and Chen (Microscale Thermophysical Engineering, 2001)

INTERFACE SCATTERING





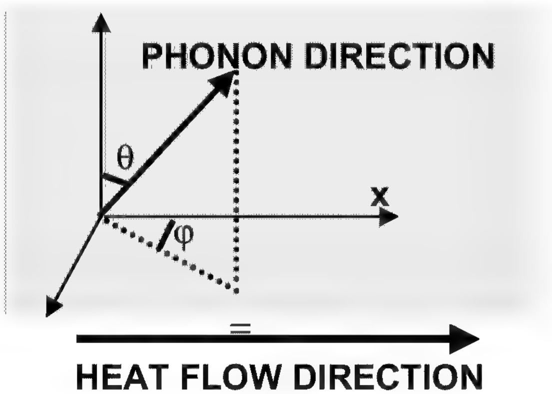
Chen, J. Heat Transf., 119, 220 (1997); Phys. Rev. B, 57, 14958 (1998).

PHONON ENGINEERING IN NANOSTRUCTURES

BULK MATERIALS $K = \frac{1}{3}\int_0^{\omega_{max}} C(\omega)v(\omega)\Lambda(\omega)d\omega$

To Reduce K in Bulk Materials: Reduce Λ (Alloys, Rattlers)

NANOSTRUCTURES $K = \frac{1}{4\pi}\int_0^{\omega_{max}} \left[\int_0^{2\pi} \sin^2\varphi d\varphi \left\langle \int_0^{\pi} C(\omega) v(\omega,\theta,\varphi)\Lambda(\omega,\theta,\varphi)\cos^2\theta \sin\theta d\theta \right\rangle \right] d\omega$



To Reduce K in Low-Dimensional Structures

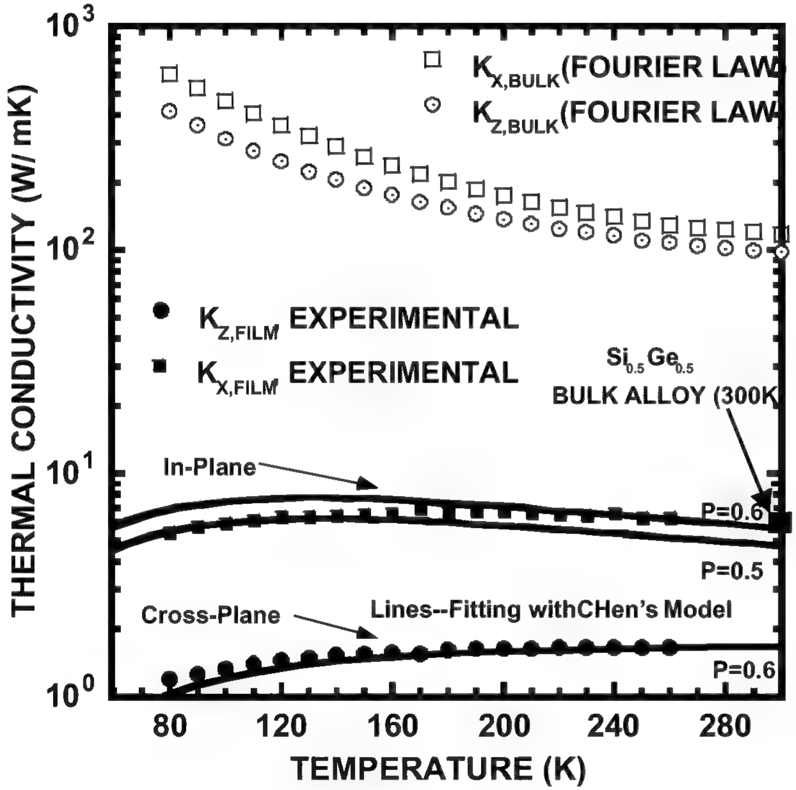
- Reduce Λ: Bulk and Interface Scattering
- Reduce V: Phonon Folding & Standing Waves
- Reduce C: Density of States Change
- Reduce Integration Limits Over Solid Angle

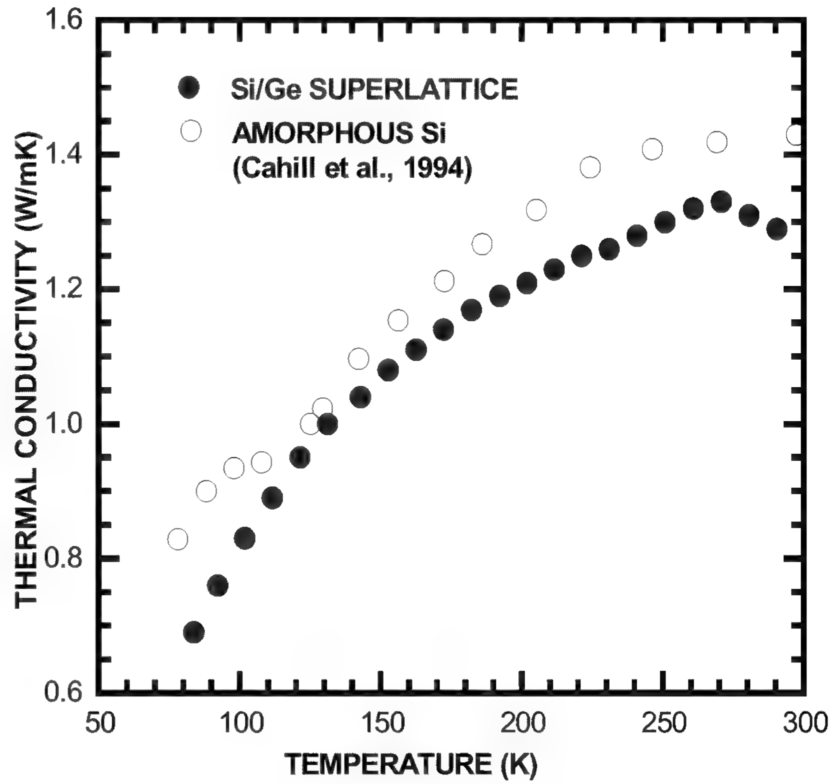
  Total Internal Reflection
- Reduce Integration Limits Over Frequency

  Phonon Confinement

Chen (Semiconductors&Semimetals, v.71, 2001)

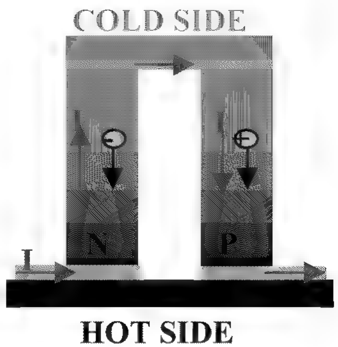
EXAMPLES





Si/Ge Superlattice

Thermoelectric Energy Conversion



Solid-State Coolers
and Power Generators

Nondimensional Figure of Merit

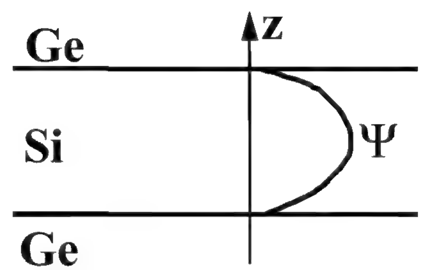
Joule Heating

Seebeck Coeff. Electron Cooling

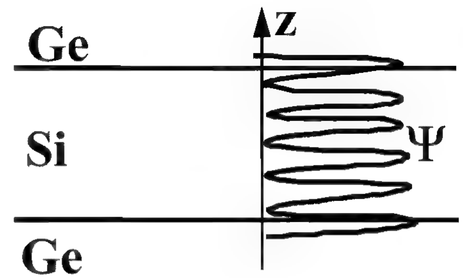
$$ZT = \frac{\sigma S^2 T}{k}$$

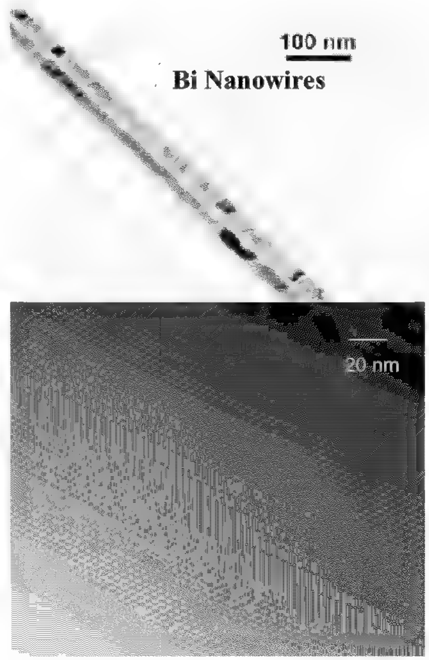
Reverse Heat Leakage Through Heat Conduction

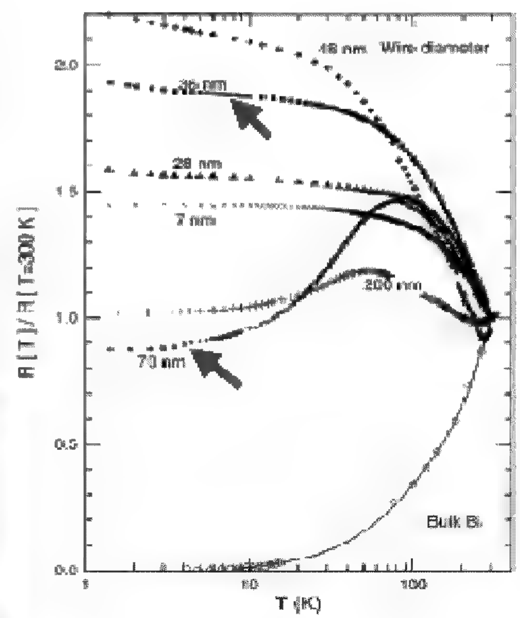
ELECTRONS



PHONONS







(Dresselhaus, Wang, et al.)

THERMAL ENGINEERING OPPORTUNITIES

Energy Technology

- Heat Conduction, k
  - Interface Scattering
  - Nanostructures
- Thermal Radiation, ε
  - Photonic Gap
  - Inhibit Thermal Emission
  - Microstructures

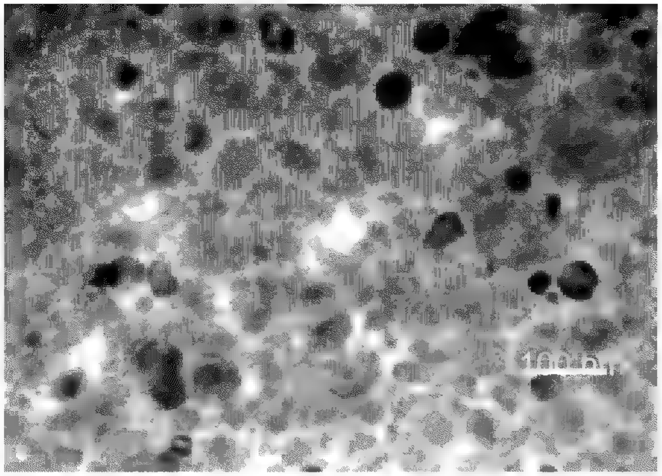
1. Porous Media Combustion
2. Phononic-Photonic Super Thermal Insulators for Coatings

Thermal+?→Technology

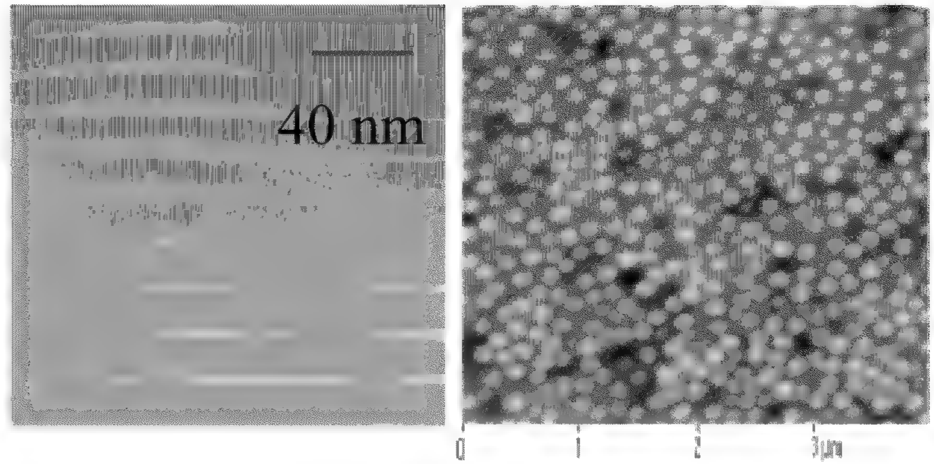
- Thermo-Electric
  - Thermoelctric
  - Thermionic
  - Microelectronics
- Thermo-Optic
  - Refractive Index
  - IR Coatings
  - Telecommunication
- Thermo-Mechanic
- Thermo-Photo-Voltaic

⋮

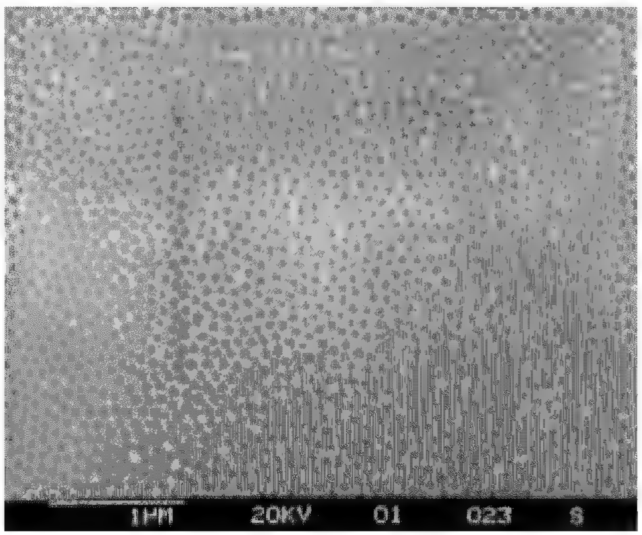
NANOSTRUCTURED THERMAL MATERIALS



NANOPOROUS BISMUTH



QUANTUM DOTS

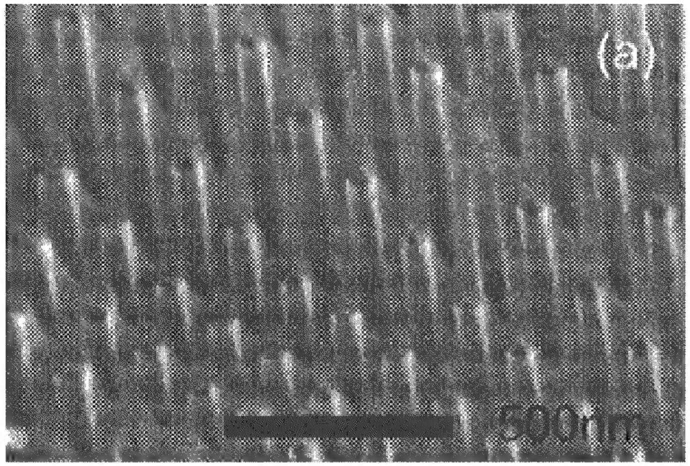


NANOCHANNELLED ALUMINA

- Low Thermal Conductivity
- Highly Anisotropic Properties

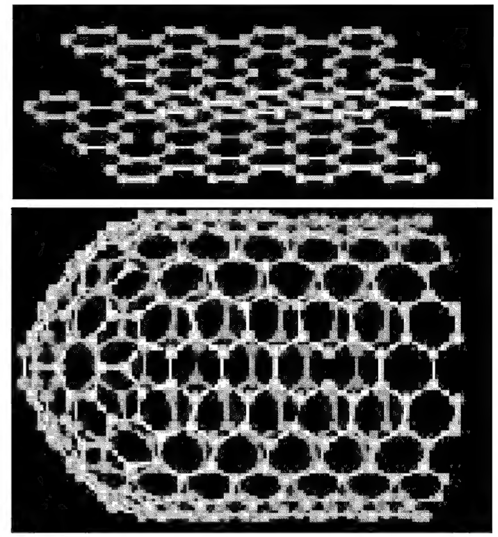
- Coatings for Engines and Turbines
- Thermal Materials for Microdevices

ENGINEERING SCATTERING



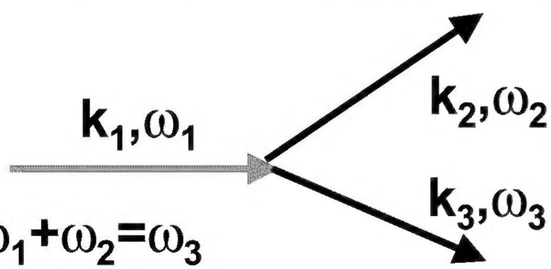
Carbon Nanotube Arrays

[from Suh and Lee, Appl. Phys. Lett., 75, 2047, 1999].



Carbon Sheet and Tubes
(http://cnst.rice.edu/pics.html)

Three-Phonon Scattering



$\omega_1+\omega_2=\omega_3$

$k_1=k_2+k_3+G$

IN A SHEET, ONLY // WAVEVECTORS

$\downarrow$

POSSIBLE TO HAVE A LARGE K

ELECTRONICS + THERMAL MANAGEMENT

HEAT CONDUCTION THEORIES

- **Fourier Law:** **Diffusion, Local Equilibrium, Infinite Speed**

$$\mathbf{q}(\mathbf{r},t) = -k\nabla T(\mathbf{r},t)$$

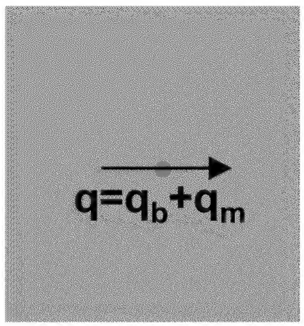
- **Cattaneo Equation:** **Diffusion, Local Equilibrium, Finite Speed**

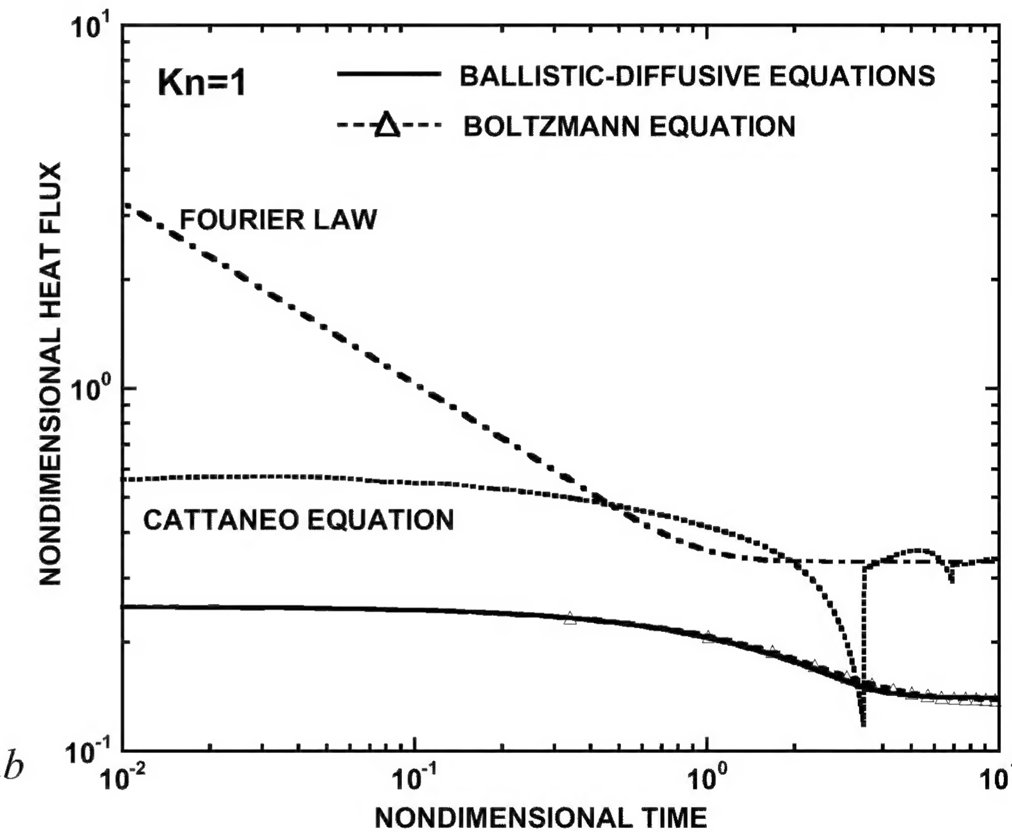
$$\tau\frac{\partial \mathbf{q}}{\partial t} + \mathbf{q}(\mathbf{r},t) = -k\nabla T(\mathbf{r},t)$$

- **Boltzmann Equation:** **Dilute Particle Transport, Phase Space**

$$\frac{\partial f(\mathbf{r},\mathbf{v},t)}{\partial t} + \mathbf{v}\bullet\nabla f = -\frac{f - f_o}{\tau}$$

BALLISTIC-DIFFUSIVE HEAT CONDUCTION EQUATIONS





q_b---originating from boundary
ballistic transport

q_m--scattered and emitted carriers
diffusive transport

$$C\left(\tau\frac{\partial^2 T_m}{\partial t^2}+\frac{\partial T_m}{\partial t}\right)=\nabla(k\nabla T_m)-\nabla\bullet\mathbf{q}_b$$

$$\mathbf{q}_b(t,\mathbf{r})=\int\left[\int I_{w\omega}\left(t-(s-s_o)/|\mathbf{v}|,\mathbf{r}-(s-s_o)\hat{\Omega}\right)\exp\left(-\int_{s_0}^{s}\frac{ds}{|\mathbf{v}|\tau_\omega}\right)\cos\theta d\Omega\right]d\omega$$

Chen, Phys. Rev. Lett., v. 86, p. 2297 (2001).

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